How to solve Schrödinger wave equation for a given wave function of a particular orbital [closed]

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Closed 7 days ago.

(Private feedback for you)

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For the wave function of $2s$ electron of a hydrogen atom, the Schrödinger wave equation, not given in my textbook is;

$$\psi_{2s} = \frac{1}{\sqrt{32\pi}}\left(\frac{1}{a_\circ}\right)^{\frac{3}{2}}\left(2 - \frac{r_\circ}{a_\circ}\right)e^{-\frac{r_\circ}{a}}$$

For 3s orbital of hydrogen atom, the normalised wave function, I found from this question

$$\Psi_{3s} = \frac{1}{81\sqrt{3\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left[27 - \frac{18r}{a_0} + \frac{2r^2}{a_0^2}\right]\mathrm{e}\,\frac{-r}{3a_0}$$

These Schrödinger equations and wave functions for $2s$ and $3s$ appear to be different from the original ones given in my textbook;

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E-U)\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E-U)\psi = 0$$

I am not familiar with basic calculus, I do not have the knowledge of differential equations. I do not understand Laplace operators, etc. My textbook states that "it is quite complex and knowledge of higher mathematics is needed to solve it; You will learn its solutions for different systems in higher classes".

But my textbook gives the equation for Hydrogen atom, HΨ = EΨ. How can I solve for $2s$ and $3s$ orbitals of a hydrogen atom from this? I have tried to search the solutions for this and for other higher orbitals also like $3s$, $3p$, $3d$ but I do not find any results. Is it very difficult to solve these; then why is are the solutions not easily available on the internet? I have found for solve these, then why is are the solutions not easily available on the internet. I have found for $2s$ and $3s$ which I have shown above. But I have no idea how it has been derived from HΨ = EΨ.

quantum-chemistry orbitals electrons atomic-structure

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edited Sep 25 at 16:04
Ian Bush
1,854 1 11 20

asked Sep 25 at 15:15
huzaifa abedeen
73 15

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5 I'm afraid from what you have said you just don't have the tools to solve the Schrodinger Equation for the hydrogen atom - at the end of my Chemistry Degree specialising in Physical and Theoretical Chemistry I would have just about been able to do it, without calculus it is impossible. Instead you will have to rely on tables - see e.g. chem.libretexts.org/Bookshelves/… – Ian Bush Sep 25 at 15:51

3 Also what you have is *not* the Schrodinger equation for the Hydrogen Atom - see chem.libretexts.org/Bookshelves/… for it in spherical coordinates. If you don't know what spherical coordinates are again this is a tool that you will need to learn to solve this equation. – Ian Bush Sep 25 at 15:55

6 Given a wave function, there is nothing to solve. The equation is already solved. This is a solution (one of many). – Ivan Neretin Sep 25 at 17:12

1 Solving the Schrödinger equation is a huge task, I remember having followed Prof. E. Bright Wilson at Harvard University, showing us how to do it rigorously for the H atom. It took him 6 hours in front of two blackboards, without losing too much time explaining what he did. I don't remember the number of times he had to change variables. In case of difficulty we had to read his book, where the solution was explained : Linus Pauling, E. Bright Wilson, Introduction to Quantum Mechanics, with Applications to Chemistry, Mc Graw-Hill, NewYork, 1935. p. 112 - 150 – Maurice Sep 25 at 19:57

2 What is exactly the question? Are you looking for a specific solution? Do you expect us to explain you the whole solution process, when you have no idea even about the basic mathematical operations in these equations? Even remotely...? – Greg Sep 26 at 10:40